

CLAIMS:

What is claimed is:

1. A method for characterizing a chemical sample, comprising:
5 obtaining a chromatogram from a series of mass spectra of said sample, wherein said mass spectra are generated by chromatography and mass spectrometry, and wherein said chromatogram comprises signal data and noise data; and applying a median filter to said chromatogram to remove at least some of said noise data, thereby producing a filtered chromatogram.
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2. The method of claim 1, wherein said chromatogram is a total ion chromatogram and said filtered chromatogram is a filtered total ion chromatogram.
3. The method of claim 2, further comprising generating individual
15 chromatograms from said total ion chromatogram, wherein said median filter is applied to said individual chromatograms.
4. The method of claim 1, wherein said median filter is a moving median filter.
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5. The method of claim 1, wherein said median filter is a modified median filter.
6. The method of claim 1, further comprising selecting a parameter of said median filter.
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7. The method of claim 6, wherein said parameter is selected in dependence on a scan rate of said mass spectrometry.
8. The method of claim 6, wherein said parameter is selected in
30 dependence on subsequent data analysis of said mass spectra.

9. The method of claim 8, wherein said subsequent data analysis comprises peak selection.

10. The method of claim 1, further comprising performing a component detection analysis on said filtered total ion chromatogram.

11. The method of claim 1, wherein said chromatography is liquid chromatography.

12. A program storage device accessible by a processor, tangibly embodying a program of instructions executable by said processor to perform method steps for a chemical sample analysis method, said method steps comprising:
obtaining a chromatogram from a series of mass spectra of said sample, wherein said mass spectra are generated by chromatography and mass spectrometry, and wherein said chromatogram comprises signal data and noise data; and
applying a median filter to said chromatogram to remove at least some of said noise data, thereby producing a filtered chromatogram.

13. The program storage device of claim 12, wherein said chromatogram is a total ion chromatogram and said filtered chromatogram is a filtered total ion chromatogram.

14. The program storage device of claim 13, wherein said method steps further comprise generating individual chromatograms from said total ion chromatogram, wherein said median filter is applied to said individual chromatograms.

15. The program storage device of claim 12, wherein said median filter is a moving median filter.

16. The program storage device of claim 12, wherein said median filter is a modified median filter.
17. The program storage device of claim 12, wherein said method steps further comprise selecting a parameter of said median filter.
18. The program storage device of claim 17, wherein said parameter is selected in dependence on a scan rate of said mass spectrometry.
19. The program storage device of claim 17, wherein said parameter is selected in dependence on subsequent data analysis of said mass spectra.
20. The program storage device of claim 19, wherein said subsequent data analysis comprises peak selection.
21. The program storage device of claim 12, wherein said method steps further comprise performing a component detection analysis on said filtered total ion chromatogram.
22. The program storage device of claim 12, wherein said chromatography is liquid chromatography.